

Criterion for bosonic superfluidity in an optical lattice

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We show that the current method of determining superfluidity in optical lattices based on a visibly sharp bosonic momentum distribution $n(\mathbf{k})$ can be misleading, for even a normal Bose gas can have a similarly sharp $n(\mathbf{k})$. We show that superfluidity in a homogeneous system can be detected from the so-called visibility (v) of $n(\mathbf{k})$ – that v must be 1 within $O(N^{-2/3})$, where N is the number of bosons. We also show that the $T = 0$ visibility of trapped lattice bosons is far higher than what is obtained in some current experiments, suggesting strong temperature effects and that these states can be normal. These normal states allow one to explore the physics in the quantum critical region.

There has been strong interest in using cold atoms in optical lattices to simulate strongly correlated many-body systems so as to shed light on many long standing problems in condensed matter physics. The interest began a few years ago with experiments on the superfluid-insulator transition of bosonic atoms in optical lattices [1], and has grown rapidly since the achievement of fermion pair condensation near a Feshbach resonance [2]. One class of very important problems, including high T_c superconductivity, is understanding how superfluid order (bosonic or fermionic) develops, and how the superfluid transforms into other correlated many-body states as the interaction parameters are varied. To achieve this goal, it is necessary to reach quantum degeneracy in a lattice, and to identify the presence of superfluidity.

At present, the method commonly used for identifying superfluidity of bosons is through the “sharpness” of the diffraction spots in their momentum distribution $n(\mathbf{k})$ [1, 3, 4, 5, 6]. Despite its popularity, there has been no effort to characterize this “sharpness” precisely. As far as we can tell, a peak is considered “sharp” if its width is visually much smaller than the separation of peaks. To be sure, a macroscopic bosonic superfluid is characterized by a δ -function peak in $n(\mathbf{k})$ (of order N where N is the number of particles). Unfortunately, the presence of such δ -function is hard to discover due to finite experimental resolution. Instead, one relies on the estimate of sharpness mentioned above, which is consistent with but not a proof of superfluid correlation, as we explain below.

The purpose of this paper is to point out a number of facts crucial for identifying superfluid order for bosons in optical lattices. We show that **(I)** even a normal Bose gas above T_c can have a diffraction pattern as sharp as those in current experiments. Identifying superfluid order from the sharpness of $n(\mathbf{k})$ as practiced today is therefore unreliable. **(II)** For homogeneous systems, the presence of superfluid order implies that the so-called “visibility” (v) must be 1 within $O(N^{-2/3})$. We also present **(III)** the visibility at $T = 0$ as a function of lattice parameters for the “wedding cake” structure of harmonically confined lattice bosons. In this case, v deviates from 1 when the superfluid regions are sufficiently small. In current exper-

iments, this typically occurs after *more than one* Mott layers have developed. Because of the high sensitivity of v to superfluid order, this visibility curve is a good calibration of temperature effects in the system. These results have strong implications for the interpretation of many current experiments, discussed at the end.

In our discussions, we shall use the identification adopted in all current experiments [1, 3, 4, 5, 6] that the observed diffraction pattern is related to the momentum distribution of the system through a ballistic expansion of the cloud (see eq.(2) below). While this has not been proven rigorously, it is consistent with the fact that the confinement energy of a Wannier state in the tight binding limit is much larger than the interaction energy [7].

(A) Normal Bose gas in a lattice: Consider an ideal Bose gas with N bosons in an optical lattice with volume Ω . The Hamiltonian is $H = \sum_i h_i$, $i = x, y, z$, $h_i = -(\hbar^2/2m)\partial_i^2 + V_o \sin^2(\pi x_i/d)$, $V_o > 0$. When V_o is sufficiently large, only the lowest band (with energies $E_{\mathbf{k}} = -2t \sum_{i=x,y,z} \cos k_i d$ and Bloch functions $\Psi_{\mathbf{k}}(\mathbf{x})$) is thermally occupied. Above the Bose condensation temperature T_c , the chemical potential μ is determined by $N/\Omega = \Omega^{-1} \sum_{\mathbf{k}}' f_B(E_{\mathbf{k}})$, where $f_B(x) = (e^{(x-\mu)/k_B T} - 1)^{-1}$, and $\sum_{\mathbf{k}}'$ is a sum over the first Brillouin Zone. At T_c , μ reaches the bottom of the band E_0 . The momentum distribution for $T > T_c$ is $n(\mathbf{q}) = \sum_{\mathbf{k}}' f_B(E_{\mathbf{k}}) |\tilde{\Psi}_{\mathbf{k}}(\mathbf{q})|^2$, where $\tilde{\Psi}_{\mathbf{k}}(\mathbf{q})$ is the Fourier transform of $\Psi_{\mathbf{k}}(\mathbf{x})$. Experimentally, one measures the *column* distribution, $N_{\perp}(\mathbf{q}_{\perp}) = \int dq_z n(\mathbf{q})$, where $\mathbf{q} = (\mathbf{q}_{\perp}, q_z)$. Since $\tilde{\Psi}_{\mathbf{k}}(\mathbf{q})$ is non-zero only when $\mathbf{q} = \mathbf{k} + \mathbf{G}$, where \mathbf{G} is a reciprocal lattice vector, and since $E_{\mathbf{k}} = E_{\mathbf{k}+\mathbf{G}}$, we have $N_{\perp}(\mathbf{q}_{\perp}) = \int dq_z f_B(E_{\mathbf{q}}) |\tilde{\Psi}_{\mathbf{q}-\mathbf{G}}(\mathbf{q})|^2$, with $\mathbf{q} - \mathbf{G}$ in the first Brillouin zone. For a narrow band, $|\tilde{\Psi}_{\mathbf{q}-\mathbf{G}}(\mathbf{q})|^2$ is a Gaussian centered at $\mathbf{q} = \mathbf{0}$ decaying on the scale $2\pi/d$. Hence $N_{\perp}(\mathbf{q}_{\perp})$ is composed of peaks centered at reciprocal lattice vectors \mathbf{G} , with the shape of the peak given entirely by the variation of $f_B(E_{\mathbf{q}-\mathbf{G}})$ around \mathbf{G} and an overall envelope given by $|\tilde{\Psi}_{\mathbf{q}-\mathbf{G}}(\mathbf{q})|^2$.

In Fig. 1(A) we show $N_{\perp}(\mathbf{q}_{\perp})$ for a lattice with one boson per site ($N/\Omega = d^{-3}$) and $V_o = 15E_R$ at a temperature $T = 1.1T_c$, where $E_R \equiv \hbar^2 \pi^2 / (2md^2)$ is a “recoil” energy. We have found numerically that in this

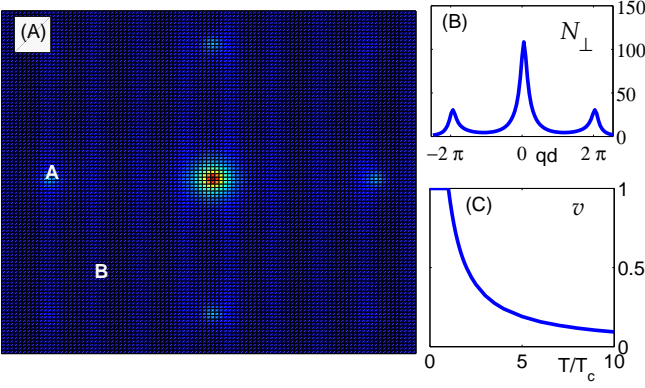


FIG. 1: (A): $N_{\perp}(\mathbf{q})$ for an ideal Bose gas with one particle per site in an optical lattice at $T = 1.1T_c$ for $V_0 = 15E_R$. A and B refer to those vectors defined in Eq. (1). (B): $N_{\perp}(\mathbf{q})$ along the q_x -axis. (C): v vs T/T_c for this ideal Bose gas.

system $k_B T_c = 0.45B$, where $B = 12t$ is the bandwidth of the lowest band, thus $k_B T < B$. As we shall see, this leads to sharp peaks distributed on a 2D square lattice with spacing $2\pi/d$. Fig. 1(B) shows that the peaks are visibly “sharp”, with a full width at half maximum $(\Delta q)_T = 0.1(2\pi/d)$. This demonstrates that *diffraction spots in $n(\mathbf{q})$ with width much less than a reciprocal lattice spacing is not proof of Bose condensation.*

(B) Condition for quantum degeneracy: The results in (A) can be understood by considering the condition for quantum degeneracy. When $k_B T < B$, the most thermally occupied states are near the bottom of the energy band, for which we can use the approximate spectrum $E_{\mathbf{k}} \approx -6t + \hbar^2 k^2 / 2m^*$, where m^* is the effective mass defined as $(m^* = \hbar^2 / (2td^2))$. The “lattice” thermal wavelength $\lambda_T = h / \sqrt{2\pi m^* k_B T}$ is reduced from the free space value $\lambda_T^{(o)}$ by $\sqrt{m/m^*}$. The condition for Bose condensation for one boson per site, which is also the condition for quantum degeneracy ($\lambda_T \sim d$), becomes $k_B T_c = 0.55B$. The difference from the numerical result ($0.45B$) is due to the effective mass approximation. The width of the spot is in general proportional to λ_T^{-1} .

Note that the change of thermal wavelength means that T_c in a lattice is reduced by a factor of m/m^* . This poses a severe challenge to reaching quantum degeneracy in the deep lattice limit. For $V_o/E_R = 10, 15, 30$, we have $m/m^* = 0.25, 0.09, 0.007$ respectively. Without lattice, for gases with 10^6 bosons in harmonic traps, T_c is typically 10^{-6}K and the lowest temperature attainable today is 10^{-9}K . For deep lattices with $m/m^* \sim 10^{-3}$, one can barely reach quantum degeneracy even at the lowest temperature attainable today [8].

(C) Visibility and Bose condensation: The visibility, originally introduced to study short range coherence[3], is defined as

$$v = \frac{N_A - N_B}{N_A + N_B}, \quad (1)$$

where $N_A = N_{\perp}(G\hat{\mathbf{x}})$, $N_B = N_{\perp}(G\hat{\mathbf{n}})$, $G = 2\pi/d$, $G\hat{\mathbf{x}}$ is a reciprocal lattice vector; $G\hat{\mathbf{n}}$ is $G\hat{\mathbf{x}}$ rotated by 45° around the $\hat{\mathbf{z}}$ axis and is not a reciprocal lattice vector. In the superfluid phase, $N_{\perp}(G\hat{\mathbf{x}}) \sim N$ while $N_{\perp}(G\hat{\mathbf{n}}) \sim N^{1/3}$ (see later discussions), so we have $v \approx 1$. The visibility of an ideal Bose gas in a lattice with $V_o = 15E_R$ and one boson per site is shown in Fig. 1(C). The visibility is 100% at $T < T_c$ but decreases sharply above T_c . It is interesting to note that despite its sharp drop at T_c , v decays slowly, remaining at 0.1 at $T = 10T_c$.

For interacting bosons in a sufficiently deep lattice, the bosons are confined to the lowest band, described by the Bose Hubbard model $H = -t \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} (a_{\mathbf{R}}^\dagger a_{\mathbf{R}'} + h.c.) + \frac{U}{2} \sum_{\mathbf{R}} n_{\mathbf{R}}(n_{\mathbf{R}} - 1)$, where $\langle \mathbf{R}, \mathbf{R}' \rangle$ means nearest neighbors, $a_{\mathbf{R}}^\dagger$ creates a boson in the Wannier state $w_{\mathbf{R}}(\mathbf{r}) = L^{-3/2} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}} \Psi_{\mathbf{k}}(\mathbf{r})$ located at site \mathbf{R} , L^3 is the number of lattice sites, and $n_{\mathbf{R}} = a_{\mathbf{R}}^\dagger a_{\mathbf{R}}$. The hopping integral t and the interaction parameter U are calculated from the eigenstates of h_i and the s-wave scattering length in a straightforward manner. Since the Fourier transform of $w_{\mathbf{R}}(\mathbf{r})$ is of the form $w_{\mathbf{R}}(\mathbf{q}) = e^{-i\mathbf{q} \cdot \mathbf{R}} w(\mathbf{q})$, the momentum distribution is

$$n(\mathbf{q}) = |w(\mathbf{q})|^2 \sum_{\mathbf{R}, \mathbf{R}'} \langle a_{\mathbf{R}}^\dagger a_{\mathbf{R}'} \rangle e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}')}. \quad (2)$$

In a homogeneous superfluid, $\langle a_{\mathbf{R}}^\dagger a_{\mathbf{R}'} \rangle$ is essentially given by $|\Psi|^2$ for $\mathbf{R} \neq \mathbf{R}'$, $\Psi = \langle a_{\mathbf{R}} \rangle$ [9]. Denoting the number of condensed bosons as $N_o \equiv L^3 |\Psi|^2$ [10], we have

$$n(\mathbf{q}) = [(N - N_o) + |\Psi|^2 f(\mathbf{q})] |w(\mathbf{q})|^2. \quad (3)$$

where $f(\mathbf{q}) = |\sum_{\mathbf{R}} e^{i\mathbf{q} \cdot \mathbf{R}}|^2$. For a narrow band, $w(\mathbf{q})$ is well approximated by $|w(\mathbf{q})|^2 = \prod_{i=x,y,z} \mathcal{W}(q_i)$, $\mathcal{W}(k) = e^{-k^2/\sigma^2} / \sqrt{\pi\sigma^2}$, $\sigma \sim 1/d$. For a cubic lattice, we have $f(\mathbf{q}) = \prod_i F(q_i)$, $F(k) = [\sin(Lkd/2)/\sin(kd/2)]^2$, which peaks sharply at reciprocal lattice vectors \mathbf{G} with a width $\sim \pi/Ld$. Since the product $\mathcal{W}(q_x)\mathcal{W}(q_y)$ has the same value at $G\hat{\mathbf{x}}$ and $G\hat{\mathbf{n}}$ and since $F(0)F(2\pi/d) = L^4$, it is simple to show from Eqs. (1) and (3) that

$$v = \frac{|\Psi|^2}{|\Psi|^2 + (N - N_o)y}, \quad y = \frac{2 \int \mathcal{W}(q_z) dq_z}{\int \mathcal{W}(q_z) F(q_z) dq_z L^4} \quad (4)$$

Simple integration shows that $y \approx \frac{d\sigma}{\sqrt{\pi}} \frac{1}{L^5}$. Since $|\Psi|^2 = N_o/L^3$, we then have *in the superfluid phase*, $v = 1 - O(1/N^{2/3})$ [11]. In order for the visibility to deviate from 1 by a non-zero but small amount, $v = 1 - \epsilon$, we need $N_o/N \sim 1/(\epsilon L^2) \sim 1/(\epsilon N^{2/3})$. Hence, even if the condensate fraction is very small, as long as it is larger than $1/(\epsilon N^{2/3})$, the visibility is essentially 1, ($1 > v > 1 - \epsilon$ to be precise). For example, a visibility of 0.95 for a system with 10^6 bosons with about a few bosons per site means $N_o/N \approx 10^{-3}$.

(D) Visibility of lattice bosons in a harmonic trap: Many recent experiments investigating quantum

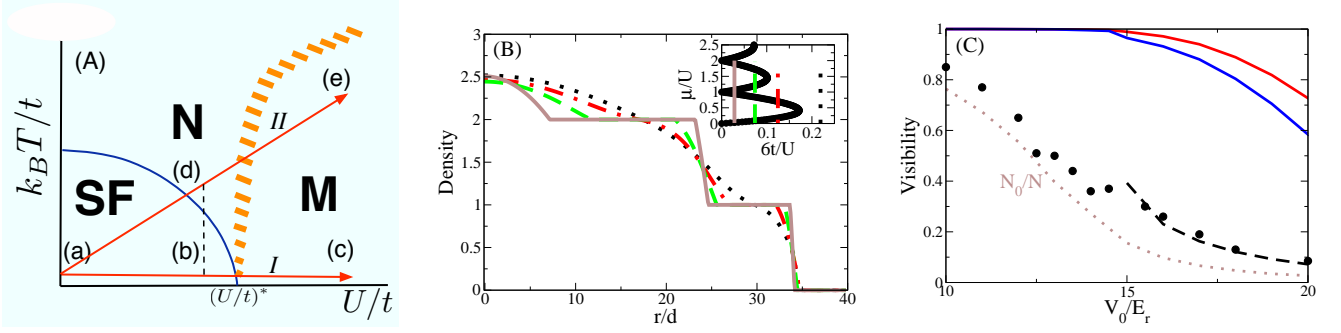


FIG. 2: (A): Schematic phase diagram for a homogenous lattice Bose gas [13]. The superfluid, (quantum critical) normal, and Mott insulator phases are labeled SF , N , and M respectively. The solid blue line is the critical temperature for the system. The shaded area is a crossover. I and II represent different physical processes. (B): Density vs radial distance for lattice bosons in a harmonic trap for conditions in ref.[14] at $V_0/E_R = 12$ (dotted black curve), 14 (dot-dashed red), 16 (dashed green), and 20 (solid brown). Inset: phase diagram for a homogeneous system. The region outside the lobes is superfluid. Vertical lines represent values taken by $\mu(\mathbf{r})$ for the corresponding V_0 . (C): $T = 0$ visibility vs V_0 . For $V_0 \leq 14.7E_R$, where the second Mott shell begins to appear, the system has a large superfluid core, which yields $v = 1$. The upper solid red (lower, solid blue) curve is the visibility when the superfluids separated by the Mott shell are in (out of) phase. The circles are experimental data from ref.[12]. The dashed line is a calculation including short range coherence assuming all superfluid regions have become Mott phases. The dotted line is the superfluid fraction at $T = 0$.

phase transitions of a lattice Bose gas or Bose-Fermi mixtures have measured the visibility of these systems in harmonic traps as a function of lattice height V_0 [3, 4, 5, 12]. Except for a single case in ref.[3] ($V_0 = 5E_R$) which finds $v = 1$ in the regime where a majority of bosons should be superfluid in the ground state, the data reported in ref.[3, 4, 5, 12] shows that $v \leq 0.8$ in a similar regime. If there was no harmonic trap, a visibility $v = 0.8$ means the lattice Bose gas is normal, as shown in Section (C). On the other hand, in a harmonic potential $V(\mathbf{r})$, it is well known that the system develops alternating layers of superfluid and Mott phases (the so-called “wedding cake” structure). When a sufficiently large number of bosons is converted from the superfluid phase to the Mott phase, the visibility will begin to drop. In addition, finite temperature or heating effects can also destroy phase coherence and reduce visibility.

To understand the general behavior of the visibility, let us consider a region in the harmonic trap (say, around \mathbf{r}) where the lattice Bose gas turns into a Mott phase as the lattice depth V_0 (and hence the ratio U/t) increases. Within the local density approximation (LDA), we can treat this region as a bulk system for which the physical process is represented as a path in the phase diagram of a homogenous lattice gas shown schematically in Fig. 2(A), which plots the transition temperature T_c as a function of U/t . At $U/t = 0$, T_c is given by the quantum degeneracy condition discussed in Section (B). It drops to zero at the quantum critical point $(U/t)^*$. The shaded line in Fig. 2(A) is the crossover from the quantum critical region (a normal phase with no clear sign of a gap) to the Mott region (a normal phase with an interaction gap).

Since experiments are performed at finite temperature, any physical trajectory connecting the superfluid phase

to the Mott phase must pass through the quantum critical region. Typically, as V_0 increases, the system heats up due to a variety of reasons : spontaneous emission, tiny vibrations of the apparatus, etc. The physical processes may therefore look like trajectories I or II shown in Fig. 2(A). The states (a) and (b) are in the superfluid phase. The final states (c) and (e) are in the Mott regime. The state (d) is in the normal regime. The proximity to a quantum phase transition can be measured by the length of the trajectory passing through the quantum critical region. For example, process I is close to the quantum phase transition, whereas II is not. In homogeneous systems, for both I and II one starts off with $v = 1$ and a sharp momentum distribution $n(\mathbf{k})$ in the superfluid region. For I , v drops sharply and $n(\mathbf{k})$ becomes blurry quickly across the transition point $(U/t)^*$. For II , v drops slowly as the system leaves the superfluid phase, and $n(\mathbf{k})$ remains sharp in the quantum critical regime close to T_c .

The proximity to a quantum phase transition can also be estimated by comparing the measured visibility to the $T = 0$ visibility calculated using standard mean field method[13] and LDA. To be concrete, we focus on the system in ref.[12] because it has the most detailed analysis of data among current experiments on lattice bosons [14]. The physics illustrated here, however, should be applicable to boson-fermion mixtures[4, 5]. We begin by calculating the order parameter $\langle a_{\mathbf{R}} \rangle = \Psi_{\mathbf{R}}$ and density $\langle n_{\mathbf{R}} \rangle$ of an infinite lattice as a function of chemical potential μ and the interaction ratio t/U for a homogeneous system. The phase boundary between superfluid and Mott phases is a sequence of “Mott lobes” as shown in the inset of Fig. 2(B). The regions within different lobes are Mott phases with different (integer) num-

ber of bosons per site. In a trap $V(\mathbf{r})$, both $\Psi_{\mathbf{R}}$ and $\langle n_{\mathbf{R}} \rangle$ are position dependent, since μ becomes (within LDA) $\mu(\mathbf{r}) = \mu - V(\mathbf{r})$. In this way, we obtain the density profiles in Fig. 2(B). (We mention that our density profiles differ from those in ref.[12], see [15]. These differences, however, will not affect our points below.) We then calculate v from Eqs. (1), (2) with $\langle a_{\mathbf{R}}^\dagger a_{\mathbf{R}'} \rangle = \langle n_{\mathbf{R}} \rangle \delta_{\mathbf{R},\mathbf{R}'} + \Psi_{\mathbf{R}}^* \Psi_{\mathbf{R}'} (1 - \delta_{\mathbf{R},\mathbf{R}'})$. If \mathbf{R} and \mathbf{R}' are in disconnected superfluid regions, the product $\Psi_{\mathbf{R}}^* \Psi_{\mathbf{R}'}$ depends on the relative phase $\Delta\theta$ between these regions.

In Fig. 2(C), we have plotted our result for v as a function of V_0 for the system in ref.[12]. The different curves correspond to different ways of treating the relative phase $\Delta\theta$ between different disconnected superfluid regions. One sees that the $T = 0$ visibility differs strongly from the experimental data (shown as circles in the figure). This large difference, however, is not due to the differences in our wedding cake structures. This is because both structures contain a superfluid core below $V_0 = 14.7E_R$ (where the second Mott shell begins to develop) that is so large that v must be 1 as long as the superfluid is not destroyed. The disagreement with experiments *implies that all superfluid regions that should exist at $T = 0$ have turned normal* (hence the much weaker visibility), which can only occur if the temperature is above T_c in these regions (i.e. the system that should be in the superfluid state (b) in Fig. 2(A) at $T = 0$ is found to be in state (d) above T_c). The physical process is therefore quite far from the quantum critical trajectory [16].

In order to account for the visibility deep in the Mott regime, the authors of ref.[12] considered short range correlations in a perturbative manner and found good agreement with their data, *provided one makes the assumption* that all the superfluid regions are converted into the Mott phase. We have repeated this procedure with our wedding cake structure [15] and have obtained similar agreement (dashed line in Fig. 2(C)). The assumption that lead to this agreement, which eliminates all contributions from superfluid to visibility, is consistent with the picture that all superfluid regions has gone normal due to temperature effects. We would like to point out that our mean field calculations do not include these short range coherence but that their inclusion would only raise the visibility curves in Fig. 2(C) to even larger values. Finally, it is instructive to look at the condensate fraction N_0/N at $T = 0$ as a function of V_0 , where $N_0 = \sum_{\mathbf{R}} |\Psi_{\mathbf{R}}|^2$. We see from Fig. 2(C) that at $T = 0$ a visibility as high as 0.8 (which occurs when $V_0 > 14.7E_R$) represents a condensate fraction $N_0/N \sim 0.05$.

(E) Implications for recent experiments: Just as in ref.[12], ref.[4, 5] also show visibility $v \sim 0.8$ for lattice heights where the system should be superfluid at $T = 0$. The physical processes in ref.[4, 5] are therefore quite far from being a quantum phase transition (QPT). (To show that a physical trajectory is close to a QPT, it is necessary to demonstrate that the quantum critical region tra-

versed in the process is very narrow). Moreover, the decrease of visibility of the bosons when fermions are added suggests that fermions may be increasing the temperature of bosons. Our discussions in Section (A) and (B) also show that the recent claim of observation of superfluid correlation of fermions in an optical lattice[6] based on the sharpness of $n(\mathbf{k})$ is not conclusive. The claim would have been established if the bosonic molecules after the sweep were found to have visibility $v = 1$.

Our study indicates that the problem of heating is prevalent in current experiments. We hope our findings will stimulate serious efforts to determine the temperature of lattice gases and more rigorous ways to achieve quantum degeneracy in lattices. This work is supported by NSF Grant DMR-0426149 and PHY-0555576.

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 - [7] The accuracy of the description of the expansion as ballistic has been reported in an experiment on a 1D lattice, P. Pedri, et.al. Phys. Rev. Lett. **87**, 220401 (2001).
 - [8] Although for a non-interacting gas the ratio T/t remains constant as the lattice is adiabatically turned on, once interactions are included this ceases to be the case.
 - [9] Strictly speaking, $\langle a_{\mathbf{R}}^\dagger a_{\mathbf{R}} \rangle$ is $|\Psi|^2$ plus a short range function $g(\mathbf{R} - \mathbf{R}')$ when $\mathbf{R} \neq \mathbf{R}'$. The latter will only change the term $N - N_0$ in eq.(3) to another quantity of the same of order but not our conclusions about the visibility.
 - [10] Due to quantum depletion, $N_0 < N$.
 - [11] The exponent $2/3$ is valid in 3D due to the integration along q_z . In 1 and 2D, $v \sim 1 - O(1/N)$.
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 - [15] In Fig. 1 of ref.[12], there is no superfluid core at $V_0 = 18E_R$. Within the same mean field and LDA, we find a superfluid core even for larger values of V_0 . We have tried to verify the cake structure in ref.[12] using their formulae for t and U but have recovered our structure instead. We also note that the results in ref.[12] are inconsistent with the parameters therein. The radii (R_1 and R_2) of the Mott layers are related to the interaction U as $U = \Delta E$, $\Delta E = \frac{1}{2}m\Omega^2(R_2^2 - R_1^2)$. Using the results in ref.[14], $R_1 = 35d$, $R_2 = 22d$, and their Ω in (see footnote [14]), we have $\Delta E = 0.62E_R$. This is 30% larger than the value obtained using their formula $U/E_R = 5.97(a/\lambda_L)(V_0/E_R)^{0.88}$, where $a = 5.45$ nm is the scattering length of ^{87}Rb .
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